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     (FILE 'WPIX' ENTERED AT 13:06:46 ON 22 SEP 2004)
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     FILE 'HCAPLUS' ENTERED AT 13:07:05 ON 22 SEP 2004
L1             1 US20040171829/PN

     FILE 'REGISTRY' ENTERED AT 13:07:11 ON 22 SEP 2004

     FILE 'HCAPLUS' ENTERED AT 13:07:14 ON 22 SEP 2004
L2             TRA L1 1- RN :       13 TERMS

     FILE 'REGISTRY' ENTERED AT 13:07:14 ON 22 SEP 2004
L3            13 SEA L2

     FILE 'WPIX' ENTERED AT 13:07:16 ON 22 SEP 2004
L4             1 US20040171829/PN

=> b hcap
FILE 'HCAPLUS' ENTERED AT 13:07:39 ON 22 SEP 2004
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FILE COVERS 1907 - 22 Sep 2004  VOL 141 ISS 13
FILE LAST UPDATED: 21 Sep 2004  (20040921/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L1   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:368618  HCAPLUS
DN   138:368624
ED   Entered STN:  14 May 2003
TI   Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic
     acids and isoxazoles.
IN   Zhou, Jiacheng; Oh, Lynette May; Ma, Philip
PA   Bristol-Myers Squibb Pharma Company, USA
SO   U.S., 20 pp.
     CODEN: USXXAM
DT   Patent
LA   English
IC   ICM  C07D295-033
     ICS  C07D241-04; C07D211-60; C07D207-06; C07C253-12
NCL  544059000; 558355000; 558309000; 544159000; 544163000; 544399000;
     546230000; 548579000
CC   25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 2
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    -------------------    --------
PI   US 6562965           B1    20030513    US 2000-610819         20000706
     US 2003208068        A1    20031106    US 2003-387759         20030313
     US 6727360           B2    20040427
     US 2004171829        A1    20040902    US 2004-786992         20040225 <--
PRAI US 1998-80680P       P     19980403
     US 1999-282508       A3    19990331
     US 2000-610819       A3    20000706
     US 2003-387759       A3    20030313
CLASS
 PATENT NO.      CLASS  PATENT FAMILY CLASSIFICATION CODES
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US 6562965 ICM C07D295-033
ICS C07D241-04; C07D211-60; C07D207-06; C07C253-12
NCL 544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
US 6562965 ECLA C07C255/41
US 2003208068 ECLA C07C253/00; C07C255/41; C07D201/08; C07D261/08; C07D261/10B
OS CASREACT 138:368624; MARPAT 138:368624
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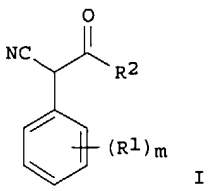
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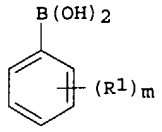
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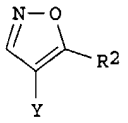
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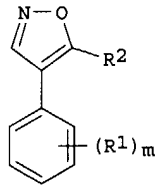
IV

AB .alpha.-Aryl-.beta.-ketonitriles [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], which serve as synthetic intermediates in the preparation of biol. important mols. such as corticotropin releasing factor (CRF) receptor antagonists, were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO3, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H2O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.

ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis

IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride
RL: CAT (Catalyst use); USES (Uses)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 246023-57-4P 246023-58-5P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole 27060-75-9, 4-Bromo-3-methylanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 7064-37-1P, 4-Bromo-5-Methylisoxazole 7064-38-2P, 4-Iodo-5-methylisoxazole 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P, 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-methoxybenzeneboronic acid 246023-55-2P 246023-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) de Munno, A; J Chem Soc, Perkin Trans 2 1977, 9, P1121 HCAPLUS
(2) Dominguez, E; J Org Chem 1966, V61, P5435
(3) Hiroyuki, Y; Chemical Abstracts 1959, V53(22)
(4) Hiroyuki, Y; Yakugaku Zasshi 1959, V79, P623
(5) Labadie, S; Synthetic Communications 1994, V24(5), P709 HCAPLUS
(6) Larock, R; Comprehensive organic transformations 1970, P57
(7) Mitchell, R; J Org Chem 1979, V44, P4733 HCAPLUS
(8) Olah, G; J Org Chem 1993, V58, P3894
(9) Olah, G; Journal of Organic Chemistry 1993, V58, P3194 HCAPLUS
(10) Rouiller, C; Heterocyclic Compounds-More than One Hetero Atom 1962, P3465
(11) Sakakibara, T; Chem Express 1989, V4, P85 HCAPLUS
(12) Sumimoto; US 4797492 A 1989 HCAPLUS
(13) Zhou; US 6107508 A 2000 HCAPLUS

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FILE 'REGISTRY' ENTERED AT 13:07:47 ON 22 SEP 2004
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STRUCTURE FILE UPDATES: 21 SEP 2004 HIGHEST RN 749178-43-6
DICTIONARY FILE UPDATES: 21 SEP 2004 HIGHEST RN 749178-43-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

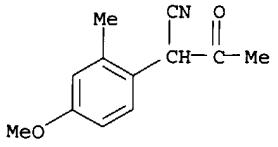
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l3 tot

L3 ANSWER 1 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **246023-58-5** REGISTRY
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2-methyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Cyano-1-(2-methyl-4-methoxyphenyl)propan-2-one
FS 3D CONCORD
MF C12 H13 N O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

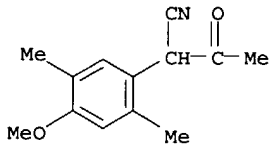


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 2 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **246023-57-4** REGISTRY
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)

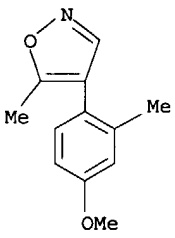
FS 3D CONCORD
MF C13 H15 N O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

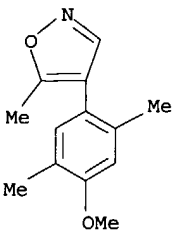
L3 ANSWER 3 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **246023-56-3** REGISTRY
CN Isoxazole, 4-(4-methoxy-2-methylphenyl)-5-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H13 N O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

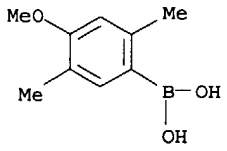
L3 ANSWER 4 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **246023-55-2** REGISTRY
CN Isoxazole, 4-(4-methoxy-2,5-dimethylphenyl)-5-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H15 N O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

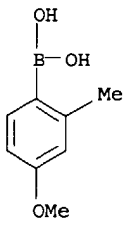
L3 ANSWER 5 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **246023-54-1** REGISTRY
CN Boronic acid, (4-methoxy-2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (4-Methoxy-2,5-dimethylphenyl)boronic acid
CN 2,5-Dimethyl-4-methoxybenzeneboronic acid
MF C9 H13 B O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 6 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **208399-66-0** REGISTRY
CN Boronic acid, (4-methoxy-2-methylphenyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Methyl-4-methoxybenzeneboronic acid
CN 2-Methyl-4-methoxyphenylboronic acid
CN 4-Methoxy-2-methylbenzeneboronic acid
CN 4-Methoxy-2-methylphenylboronic acid
MF C8 H11 B O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

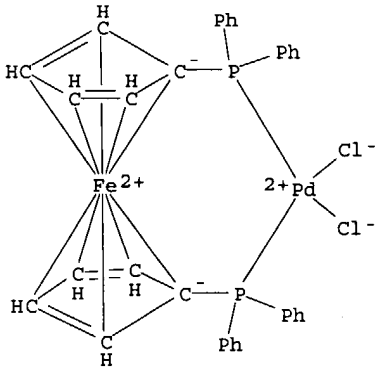


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

27 REFERENCES IN FILE CA (1907 TO DATE)
27 REFERENCES IN FILE CAPLUS (1907 TO DATE)

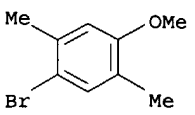
L3 ANSWER 7 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **72287-26-4** REGISTRY
CN Palladium, [1,1'-bis(diphenylphosphino-.kappa.P)ferrocene]dichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ferrocene, 1,1'-bis(diphenylphosphino)-, palladium complex
CN Palladium, [1,1'-bis(diphenylphosphino)ferrocene-P,P']dichloro-, (SP-4-2)-

OTHER NAMES:
CN (1,1'-Bis(diphenylphosphino)ferrocene)dichloropalladium
CN (Bis(.eta.5-(diphenylphosphino)cyclopentadienyl)iron)dichloropalladium
CN 1,1'-Bis(diphenylphosphino)ferrocenepalladium dichloride
CN Dichloro(diphenylphosphinoferrocene)palladium
CN Dichloro[1,1'-bis(diphenylphosphine)ferrocene]palladium(II)
CN Dichloro[1,1'-bis(diphenylphosphino)ferrocene]palladium
CN Dichloro[1,1'-bis(diphenylphosphino)ferrocene]palladium (II)
CN PdCl2(dppf)
CN [1,1'-Bis(diphenylphosphino-.kappa.P)ferrocene]dichloropalladium
DR 118588-97-9
MF C34 H28 Cl2 Fe P2 Pd
CI CCS, COM
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, GMELIN*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



469 REFERENCES IN FILE CA (1907 TO DATE)
470 REFERENCES IN FILE CAPLUS (1907 TO DATE)

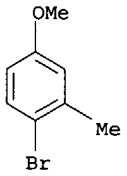
L3 ANSWER 8 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **58106-25-5** REGISTRY
CN Benzene, 1-bromo-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Anisole, 4-bromo-2,5-dimethyl- (6CI)
OTHER NAMES:
CN 1-Bromo-4-methoxy-2,5-dimethylbenzene
CN 2,5-Dimethyl-4-bromo anisole
CN 4-Bromo-2,5-dimethylanisole
FS 3D CONCORD
MF C9 H11 Br O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

24 REFERENCES IN FILE CA (1907 TO DATE)
24 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L3 ANSWER 9 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **27060-75-9** REGISTRY
CN Benzene, 1-bromo-4-methoxy-2-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Anisole, 4-bromo-3-methyl- (6CI, 8CI)
OTHER NAMES:
CN 1-Bromo-2-methyl-4-methoxybenzene
CN 1-Bromo-4-methoxy-2-methylbenzene
CN 2-Bromo-5-methoxytoluene
CN 3-Methyl-4-bromoanisole
CN 4-Bromo-3-methylanisole
FS 3D CONCORD
MF C8 H9 Br O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



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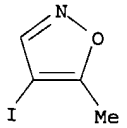
128 REFERENCES IN FILE CA (1907 TO DATE)
128 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L3 ANSWER 10 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **7064-38-2** REGISTRY
CN Isoxazole, 4-iodo-5-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-Iodo-5-methyl-1,2-oxazole
CN 4-Iodo-5-methylisoxazole
FS 3D CONCORD
MF C4 H4 I N O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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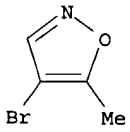
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L3 ANSWER 11 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **7064-37-1** REGISTRY
CN Isoxazole, 4-bromo-5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-Bromo-5-methylisoxazole
FS 3D CONCORD
MF C4 H4 Br N O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L3 ANSWER 12 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **5765-44-6** REGISTRY
CN Isoxazole, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 5-Methylisoxazole
CN NSC 52269
FS 3D CONCORD
DR 264871-06-9
MF C4 H5 N O
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
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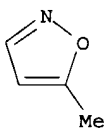
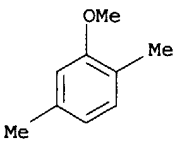
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PROC (Process); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

158 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
159 REFERENCES IN FILE CAPLUS (1907 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L3 ANSWER 13 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN **1706-11-2** REGISTRY
CN Benzene, 2-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Anisole, 2,5-dimethyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 2,5-Dimethylanisole
CN 2,5-Dimethylphenol methyl ether
CN 2-Methoxy-1,4-dimethylbenzene
CN 2-Methoxy-p-xylene
CN 3,6-Dimethylanisole
CN Methoxy-p-xylene
FS 3D CONCORD
DR 92415-84-4
MF C9 H12 O
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, HODOC*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent; Report
RL.P Roles from patents: FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FILE LAST UPDATED: 20 SEP 2004 <20040920/UP>
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AN   2000-013038 [01]   WPIX
CR   1998-159109 [14]; 1999-479164 [40]; 2004-019646 [02]
DNC  C2000-002407
TI   Preparation of alpha-aryl-beta-ketonitriles and new intermediates.
DC   B03 B05
IN   MA, P; OH, L M; ZHOU, J
PA   (DUPO) DU PONT PHARM CO; (DUPO) DUPONT PHARM CO; (MAPP-I) MA P; (OHLM-I)
     OH L M; (ZHOU-I) ZHOU J; (BRIM) BRISTOL-MYERS SQUIBB PHARMA CO
CYC  45
PI   WO 9951568      A2 19991014 (200001)* EN   64    C07C253-00
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     US 6107508      A  20000822 (200042)              C07C253-00
     BR 9909427      A  20001121 (200065)              C07C253-00
     NO 2000004956   A  20001101 (200067)              C07C253-00
     EP 1066250      A2 20010110 (200103)  EN          C07C253-00
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     CZ 2000003519   A3 20010815 (200157)              C07C253-00
     SK 2000001443   A3 20010911 (200159)              C07C253-00
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     MX 2000009659   A1 20010301 (200170)              C07C253-00
     HU 2001001798   A2 20011128 (200209)              C07C253-00
     ZA 2000004654   A  20011224 (200212)        91    C07C000-00
     JP 2002510670   W  20020409 (200227)        69    C07C253-00
     US 2003208068   A1 20031106 (200374)              C07D279-12
     US 6727360      B2 20040427 (200429)              C07D417-04
     US 2004171829   A1 20040902 (200458)              C07D279-12     <--
ADT  WO 9951568 A2 WO 1999-US6822 19990329; AU 9932135 A AU 1999-32135
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     2000004956 A WO 1999-US6822 19990329, NO 2000-4956 20001002; EP 1066250 A2
     EP 1999-914246 19990329, WO 1999-US6822 19990329; CN 1296473 A CN
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     Provisional US 1998-80680P 19980403, Div ex US 1999-282508 19990331, Div
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     JP 2002510670 W Based on WO 9951568; US 2003208068 A1 Div ex US 6107508,
     Div ex US 6562965; US 6727360 B2 Div ex US 6107508, Div ex US 6562965; US
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PRAI US 1998-80680P       19980403; US 1999-282508       19990331;
     US 2000-610819       20000706; US 2003-387759       20030313;
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IC   ICM  C07C000-00; C07C253-00; C07D000-00; C07D279-12; C07D417-04
     ICS  C07C255-40; C07D207-04; C07D211-06; C07D211-60; C07D241-04;
          C07D261-06; C07D261-08; C07D265-30; C07D279-10; C07D413-04
ICA  C07B061-00
AB   WO   9951568 A UPAB: 20040910
     NOVELTY - Preparation of alpha -aryl- beta -ketonitriles (I) is new.
          DETAILED DESCRIPTION - Preparation of alpha -aryl- beta -ketonitriles
     (I) by reaction of optionally substituted benzene with a halogenating
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agent to form an optionally substituted halo-benzene compound, reacting the product with a strong base and an alkyl borate, contacting the resulting product with a halo substituted isoxazole in the presence of a catalyst and a weak base and then contacting the product with an isomerization base to form a compound (I) or its salt.
r = 0-4;
R1 = H, 1-10C alkyl, 2-10C alkenyl, 2-10C alkynyl, 3-6C cycloalkyl, 4-12C cycloalkylalkyl, NR1cR1d, OR1e or SR1e;
R1c, R1d = H, 1-10C alkyl, 2-10C alkenyl, 2-10C alkynyl, 3-6C cycloalkyl or 4-12C cycloalkylalkyl;
Or NR1cR1d = a heterocyclic ring selected from piperidine, pyrrolidine, piperazine, N-methylpiperazine, morpholine or thiomorpholine, each heterocyclic ring optionally substituted by 1-3 (1-4C)alkyl groups;
R1e = H, 1-10C alkyl, 3-6C cycloalkyl or 4-6C cycloalkylalkyl;
R2 = H, 2-4C alkenyl, 2-4C alkynyl, 3-6C cycloalkyl, 4-10C cycloalkylalkyl, 1-4C hydroxyalkyl, 1-4C haloalkyl or 1-4C alkyl substituted by 0-5 R2a groups;
R2a = H, 1-10C alkyl, 2-10C alkenyl, 2-10C alkynyl, 3-6C cycloalkyl, 4-12C cycloalkylalkyl, halo, CN, 1-4C haloalkyl, OR2e or SR2e;
R2e = H, 1-10C alkyl, 3-6C cycloalkyl or 4-6C cycloalkylalkyl.
Preparation comprises:
(a) contacting an optionally substituted benzene (II) with a halogenating agent to form a compound (III);
(b) contacting the compound (III) with a strong base followed by the addition of an alkylborate to form a compound (IV);
(c) contacting compound (IV) with a compound (V) in the presence of a catalyst and a weak base to form a compound (VI);
(d) contacting compound (VI) with an isomerization base to form a compound (I) or a salt thereof.
X = a halogen derived from the halogenating agent;
Y = a second halogen.
INDEPENDENT CLAIMS are also included for the following:
(1) Preparation of a compound (V) comprises contacting a compound (VII) with a halogenating agent in an organic acid;
(2) a compound (VI);
(3) a compound (I).
USE - (I) are synthetic intermediates for the preparation of a series of biologically important molecules such as corticotropin releasing factor (CRF) receptor antagonists.
Dwg.0/0
FS CPI
FA AB; GI; DCN
MC CPI: B07-D03; B07-D05; B07-D11; B07-E01; B07-E03; B07-F02; B10-A15

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